2-Benzyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine
368441-96-7 | DTXSID50364048

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.63 days

Global applicability domain: Outside

Local applicability domain index: 3.84e-01

Confidence level: 8.30e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Dimethyl-4-ethylbenzene
Measured: 24.3
Predicted: 3.89

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2-Ethyl-p-xylene
Measured: 12.5
Predicted: 3.70

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1-Ethyl-2,3-dimethylbenzene
Measured: 61.9
Predicted: 4.15

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Isobutylbenzene
Measured: 201
Predicted: 6.97

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3-Methylindene
Measured: 12.5
Predicted: 2.76